Half-Integer Filling Factor States in Quantum Dots

A. Harju,[1,*] H. Saarikoski,[2,1] and E. Räsänen[3,1]

[1] Laboratory of Physics, Helsinki University of Technology, P.O. Box 1100, FI-02015 HUT, Finland
[2] Kavli Institute of NanoScience, Delft University of Technology, 2628 CJ Delft, the Netherlands
[3] Institut für Theoretische Physik, Freie Universität Berlin, Arnimallee 14, D-14195 Berlin, Germany

(Dated: February 6, 2008)

Emergence of half-integer filling factor states, such as ν=5/2 and 7/2, is found in quantum dots by using numerical many-electron methods. These states have interesting similarities and differences with their counterstates found in the two-dimensional electron gas. The $\nu = 1/2$ states in quantum dots are shown to have high overlaps with the composite fermion states. The lower overlap of the Pfaffian state indicates that electrons might not be paired in quantum dot geometry. The predicted $\nu = 5/2$ state has high spin polarization which may have impact on the spin transport through quantum dot devices. PACS: 71.10.-w, 73.21.La, 73.43.-f, 85.35.Be

The fractional quantum Hall state at filling factor $\nu = 5/2$ in the two-dimensional electron gas (2DEG) is widely thought to be a Moore-Read state of p-wave paired electrons with unusual topological properties [1]. The state has recently attracted much theoretical interest together with other half-integer filling factor states, mainly due to proposals for using it in quantum computing [2]. The 2DEG $\nu = 5/2$ state is expected to consist of two Landau levels (LL), where the filled lowest LL (0LL) is spin-compensated and the half-filled next LL (1LL) is spin polarized state described by a Pfaffian (PF) wave function [3]. This wave function explicitly describes the electron pairing which is analogous to that in the BCS theory of superconductivity. Due to the half-filling of 1LL at $\nu = 5/2$, the properties of the $\nu = 5/2$ state is usually analyzed using the $\nu = 1/2$ state with an interaction Hamiltonian corrected for the screening effects of the electrons in the filled 0LL.

Unlike half-integer filling factor states in the 2DEG, the corresponding states in quantum dots (QD's) have got almost no attention until now (see Ref. 4 for an exception). In this Letter we analyze the electronic structure of QD's in magnetic fields and find new states which can be regarded as finite size counterparts of the half-integer filling factor states in the 2DEG. Since the emergence of fractional quantum Hall states is always a result of electron-electron interactions, we use numerical methods which can take into account the complex correlation effects in the system. The results indicate analogies but also important differences between the states in the half-integer filling factor range in the 2DEG and QD's. The mean-field method predicts that due to the presence of an external confining potential in QD's, the $\nu = 5/2$ state appears as a mixture of $\nu = 2$ and 3. We analyze also the internal structure of the many-body state at $\nu = 1/2$ in QD's and compare it to the PF wave function and the composite fermion (CF) model [5]. Unlike the CF model, which yields high overlaps with the exact state, the PF wave function is found to poorly describe the pure $\nu = 1/2$ state and also the excited 1LL of the $\nu = 5/2$ state in QD's. Therefore, we find no evidence of electron pairing near half-integer LL fillings in QD's. We finally discuss the impact of the $\nu = 5/2$ state on the ground state energetics and on the spin transport through the QD and find that signatures of this state can be found, e.g., in magnetization measurements or electron tunneling experiments.

We define our QD system by an effective-mass Hamiltonian for N electrons

$$H = \sum_{i=1}^{N} \left[\frac{(\mathbf{p}_i + e\mathbf{A})^2}{2m^*} + V_c(r_i) + g^* \mu_B S_{z,i} \right] + \sum_{i<j} \frac{e^2}{4\pi\epsilon r_{ij}} \, ,$$

with material parameters for GaAs, i.e, $m^* = 0.067$, $\epsilon/\epsilon_0 = 12.4$, and $g^* - 0.44$. Unless stated otherwise, we apply a parabolic confining potential, $V_c(r) = m^*\omega_0^2 r^2/2$ with a strength $\hbar\omega_0 = 5.7N^{-1/7}$ meV. The N dependence in ω_0 is introduced to keep the electron density in the dot approximately constant. We solve the associated Schrödinger equation using the mean-field spin-density functional theory (SDFT) and the exact diagonalization (ED) method [6]. We use the SDFT to calculate the electronic structure of large quantum dots which are beyond reach of exact many-body method. The internal structure of the half-filled LL is then analyzed in detail with the ED method which is, however, restricted to fairly low electron numbers.

We analyze the polarization and occupations of the LL's in large QD's using the SDFT. We focus here on the filling factor regime $\nu \geq 2$. One finds that the filling factor for the finite electron systems is position dependent [7]. Even at integer filling factors (where most physics can be understood on a single-particle level), the 2DEG and QD's have differences due to the overlapping of LL's in QD's in low magnetic fields. In QD's we identify the integer ν as states, where the increasing magnetic field has emptied one of the LL's completely of electrons. For example, $\nu = 3$ corresponds to case where magnetic field has emptied 2LL and the spin-compensated 1LL has approximately one third of the electrons, the rest being at 0LL. In the 2DEG, 1LL is spin split at $\nu = 3$ and has one spin channel fully occupied.

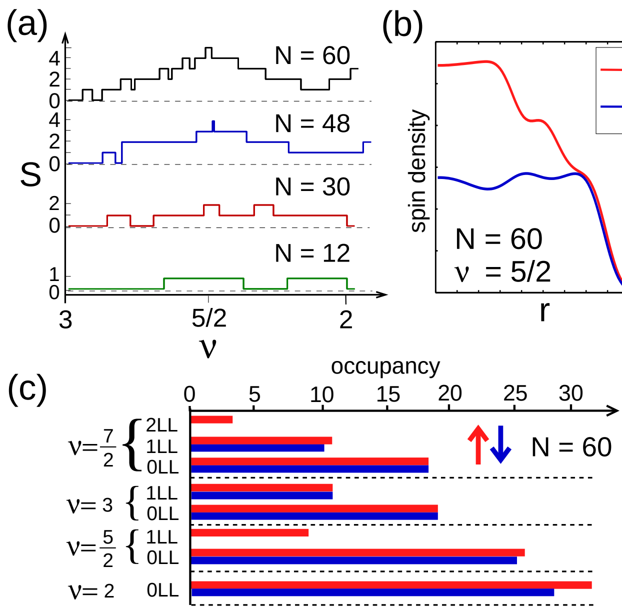

FIG. 1: (color online) (a) Ground-state spin of quantum dots with $N = 12$, 30, 48, and 60 electrons, respectively. The magnetic fields are scaled linearly to filling factor range $2 \leq \nu \leq 3$. (b) Spin densities of the $N = 60$ quantum dot at $\nu = 5/2$. The spin-polarized second Landau level gives rise to high spin polarization in the core region of the dot. (c) Occupation of the single-electron (Kohn-Sham) states on different Landau levels in the $N = 60$ quantum dot at $2 \leq \nu \leq 7/2$.

Figure 1(a) shows the calculated spin polarization $S = (N^{\uparrow} - N^{\downarrow})/2$ of the ground state of QD's with $N = 12$, 30, 48, and 60 electrons, respectively. Our starting point is the $\nu = 3$ state discussed above. When the magnetic field is increased electrons move from 1LL to 0LL. This occurs mainly for spins anti-parallel to the magnetic field. We find a peak in S between $\nu = 2$ and $\nu = 3$ where all the spins anti-parallel to the magnetic field have fallen to 0LL leaving 1LL totally spin polarized with angular momentum states $l = -1, 0, 1, \ldots, n_{1\mathrm{LL}} - 2$. Since the spin polarization of 1LL agrees with the expected spin polarization of the Moore-Read state in the 2DEG, we identify this state as a finite-size counterpart of $\nu = 5/2$. In addition, $\nu_{\mathrm{avg}} = 2.54$ (see Ref. 7) for this state when $N = 60$. The spin density of $\nu = 5/2$ state at $N = 60$ shows that the spin polarization is concentrated at the core of the dot [Fig. 1(b)]. This result is in contrast with the structure of the 2DEG where the single-particle states on 1LL are uniformly occupied, whereas in QD's the occupation has a compact structure due to the external confinement. Thus, the $\nu = 5/2$ state in QD's can be interpreted to be composed of two different filling factor domains, i.e., $\nu = 2$ at the edge and $\nu = 3$ at the center. We find also an analogous state in lower magnetic fields $\nu > 3$ where the 2LL is spin polarized. We identify this state as $\nu = 7/2$. The Kohn-Sham occupations of LL's for $\nu = 2$, $5/2$, 3, and $7/2$, respectively, show the mechanism of LL filling in QD's [Fig. 1(c)]. Due to partial filling of 1LL, the $\nu = 3$ state can also be interpreted as a combination of $\nu = 2$ and $\nu = 4$ states.

Increasing the magnetic field beyond $\nu = 5/2$ forces the spin-polarized electrons in 1LL to fall one-by-one down to 0LL, starting from the electrons with highest angular momenta. 1LL maintains the spin polarization but the electrons in 0LL tend to prefer spin compensated configuration and, as a consequence, there is a partial relapse towards lower total spin polarization. However, near $\nu = 2$ 0LL gets a small spin polarization in high electron numbers, e.g., $S = 1$ for $N = 48$ and $S = 2$ for $N = 60$ [see Fig. 1(a)]. This result is in accord with the results of Ciorga and coworkers who found the collapse of the spin singlet state in large QD's at $\nu = 2$ (Ref. 9).

The results at $\nu = 5/2$ can be generalized to larger particle numbers by assuming a spin compensated 0LL and polarized 1LL. The formula of $\nu_{0\mathrm{LL}}$ (see Ref. 7) gives $S \approx N/10$ for the spin polarization at $\nu = 5/2$, which is in a reasonable agreement with the calculated maximum spin polarization of the two largest dots in Fig. 1(a). As seen above in the case of $\nu = 7/2$, we find also evidence of analogous polarization of the highest occupied LL in lower magnetic fields. This suggests that the results can be generalized to higher half-integer filling factor states ($\nu = 9/2$ etc.) in sufficiently large QD's.

The predicted spin polarization of the states between $2 \leq \nu \leq 3$ is interesting with a viewpoint on the spintronics in which electron spin degree is exploited to create novel device concepts and new functionality for electronic circuits. It is assumed that the alternation of states in the $2 < \nu < 3$ regime leads to the familiar checkerboard pattern of conductance peak heights in the electron tunneling through a QD device [10, 11]. However, the details of the current patterns are not completely understood. The checkerboard behavior is usually explained assuming oscillations between the spin singlet $S = 0$ and triplet $S = 1$ states [12] which can be qualitatively modeled within the constant-interaction picture [13] with a phenomenological exchange term. Our SDFT calculations indicate that this model is sufficiently accurate in low electron numbers [see, e.g., data for $N = 12$ in Fig. 1(a)], but there are significant deviations from it for $N \geq 20$. The constant-interaction model cannot take into account the correlation effects which give rise to the high spin polarization near the $\nu = 5/2$ state in large QD's. This might affect electron tunneling probability through the dot for high electron numbers and, as a consequence, leave a trace to the pattern of conductance peak heights. However, the high probability transmission in the experiments occurs mainly through the edge region which is not spin polarized [10]. The transport through the center of the dot gives rise to lower conductance peak heights, and evolution of the ground state spin might leave a systematic pattern in the low probability transmission peak heights.

We turn now into analysis of the exact many-body

wave function of the $\nu = 1/2$ state. We use the ED method on 0LL, and the results are compared to two models, the PF and the CF wave functions [5]. The PF wave function [1] is defined as

$$\Psi_{\rm PF} = {\rm Pf}\left(\frac{1}{z_i - z_j}\right)\prod_{i<j}(z_i - z_j)^2 \exp\left(-\frac{1}{2}\sum_i r_i^2\right) \ ,$$

with angular momentum $L = N(N-1) - N/2$. The value of the filling factor at $\nu < 1$, i.e., beyond the maximum-density-droplet (MDD) domain is widely approximated to be $\nu_{\rm J} = L_{\rm MDD}/L$. This definition is based on Jastrow states but the PF wave function has $\nu_{\rm J}$ which is slightly higher than 1/2. As the number of particles in the system increases, $\nu_{\rm J}$ for the PF approaches 1/2 from above as $\nu_{\rm J} = 1/2 + 1/2N + O(1/N)^2$. The PF state is constructed for even N, and we are computationally limited to $N \le 8$. The CF wave functions [5] used here are defined as

$$\Psi_{\rm CF} = \exp\left(-\frac{1}{2}\sum_i r_i^2\right)\Psi_0 \prod_{i<j}(z_i - z_j)^2 \ ,$$

where Ψ_0 is a determinant formed from the single-particle states $\psi_{n,l} \propto z^{n+l}\partial^n$, with l the angular momentum and $n = 0, 1, 2\ldots$ is the LL index. The derivative is with respect to z, and the resulting many-body state has a total angular momentum $L = N(N-1) + \sum_{i=1}^{N} l_i$.

There are several possibilities for the single-particle occupations in Ψ_0 for the states near $\nu_{\rm J} \approx 1/2$. We consider two different CF wave functions: CF1 that have the same angular momentum as PF states, and CF2 that have $\nu_{\rm J} = 1/2$, so that $L = N(N-1) = 2L_{\rm MDD}$. The first type have single-particle quantum numbers (n, l) of the occupied states as $(0, i-1)$ and $(i, -i)$, $i = 1, \ldots, N/2$, and in the second one the asymmetry in l quantum numbers is recovered by moving a particle from $(N/2, -N/2)$ to $(1, 0)$. The CF2 wave function is constructed also for odd N. The numerical projection to 0LL (derivatives in Ψ_0) is doable up to $N = 6$. From these wave functions, CF1 (and thus also PF) has an angular momentum that corresponds to the ground-state of $N = 4$, and CF2 for $N = 5$ and 6. In Table I we show the accuracy of the three wave functions discussed above. PF is clearly less accurate than CF which has very high overlaps. The reasonably high overlap (around .6) means, however, that PF cannot be an accurate excited state. Therefore we find no evidence of electron pairing in the $\nu = 1/2$ state.

Figure 2 shows the conditional wave functions [6], obtained by fixing $N-1$ electrons and moving the remaining electron, for the PF and corresponding ED state. One can see that the most probable positions are different in ED and PF and the ED conditional density is more localized than the PF one.

In the 2DEG the electrons in the half-filled 1LL can be described by a $\nu = 1/2$ state on 0LL having a screened electron-electron interaction. This state is accurately modeled using a PF wave function [1, 3]. The mean-field results above suggest that because of the different structure of the $\nu = 5/2$ states in QD's and the 2DEG systems, the $\nu = 5/2$ state is not related to $\nu = 1/2$ in parabolically confined QD's. The 1LL in QD's is compact and does not have the required angular momentum of the $\nu = 1/2$ state. One might assume that realistic inter-electron potentials, which are modified by screening from the electrodes and finite thickness of the sample, would induce electron pairing as observed in numerical studies of the $\nu = 5/2$ state in the 2DEG. However, ED calculations with a screened electron-electron interaction indicate that overlaps of the PF with the exact state increases only marginally. Therefore we find no evidence of electron pairing in the analyzed half-integer filling factor states in QD's confined by a parabolic external potential.

TABLE I: Overlaps of the trial wave functions with exact one for different particle number N.

N	PF	CF1	CF2
4	0.922124	0.999903	0.997978
5	-	-	0.998921
6	0.789996	0.993461	0.996096
8	0.586370	-	-

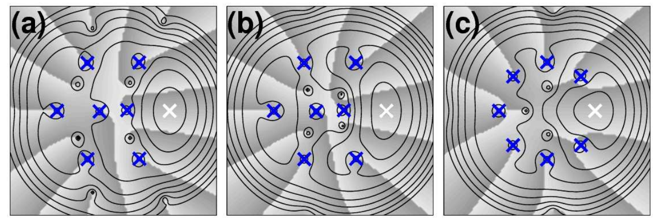

FIG. 2: (color online) Electron positions (crosses), conditional electron densities (contours), and phases (gray-scale) of the $N = 8$, $L = 52$ state from ED (a) and PF model (b and c). We probe with the rightmost electron and densities are on logarithmic scale. The phase changes from π to $-\pi$ on the lines where the shadowing changes from the darkest gray to the white. In (a) and (c) electrons are on the most probabe positions, and in (b) we use ED coordinates for PF.

The confinement potential in actual QD's may vary considerably from the parabolic shape [14]. However, this fact seem not to affect notably the appearance of the $\nu = 5/2$ state in QD's. Our SDFT calculations for a 60-electron QD defined by an infinite potential well of radius 150 nm yield the $\nu = 5/2$ state similarly to the parabolic case. As the main difference, the state is not separated into two $\nu = 2$ and $\nu = 3$ domains in the infinite-well QD. Instead, electrons on 0LL are strongly localized near the edge, whereas the spin-up electrons on 1LL contribute in the mid-region leaving the electron density in the core relatively flat for both spin types. In the ground-state energetics the behavior between different QD's is similar,

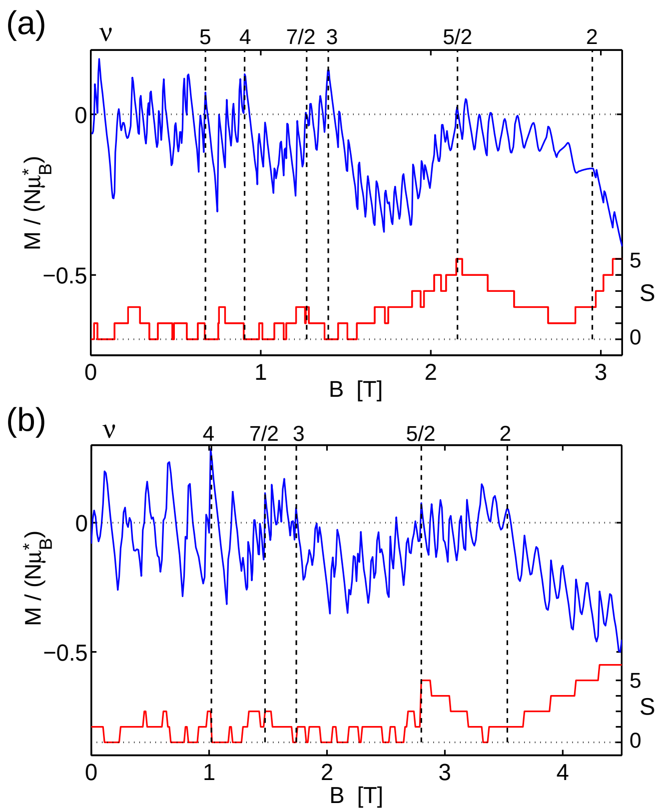

FIG. 3: (color online) Ground-state magnetization (upper curves) and total spins (lower curves) of 60-electron quantum dots in parabolic (a) and infinite-well (b) potentials. The finite size counterparts of the integer and fractional quantum Hall states are marked in the figures (dashed lines).

as we demonstrate in Fig. 3 showing the SDFT result of the magnetization, $M = -\partial E_{\rm tot}/\partial B$, for 60-electron parabolic and infinite-well QD's, respectively. The peaks in M coincide with the integer filling factors and constitute the finite size counterpart of the de Haas–van Alphen effect. In both cases, the $\nu = 5/2$ state leaves cusps in the magnetization, and the data shows also possible development of other half-integer filling-factor states such as $\nu = 7/2$ in lower magnetic fields. The results are consistent with the few direct magnetization measurements of ensembles of large QD's which have shown a cusp-like structure near $\nu = 5/2$ (Ref. 15). Visible signatures are also expected to be found in the chemical potentials of electron tunneling experiments.

To conclude, we predict emergence of states in quantum dots which can be regarded as finite size counterparts of the half-integer filling factor states in the 2D electron gas. The highest occupied Landau level of these states is found to be spin-polarized and the formation of them leaves signatures in the ground state energetics. The numerical results indicate that these states share many of the characteristics of their infinite size counterparts in the 2D electron gas, although we find also major differences. Due to observed stability of these states we postulate that the formation of them is a general property of finite fermion systems in external confinement. In parabolic confining potential the composite fermion picture is found to be a more accurate description of the $\nu = 1/2$ state than the Pfaffian wave function, which suggests that electrons are not paired in this geometry. The electron pairing, which is predicted to occur in the two-dimensional electron gas, might be recovered in quantum dots in the limit of very large electron numbers and with a weak non-parabolic external confinement potential.

We thank S. Siljamäki for the CF wave function code, and J. Suorsa, G. E. W. Bauer, M. Schwarz, S. Reimann and D. Grundler for fruitful discussions. This work was supported by the Academy of Finland through the Centre of Excellence Program (2000-2011) and by the NANOQUANTA NOE and the Finnish Academy of Science and Letters, Vilho, Yrjö and Kalle Väisälä Foundation (to E. R.).

* Electronic address: ari.harju@hut.fi

[1] N. Read, Physica B **298**, 121 (2001).
[2] M. Freedman, C. Nayak, and K. Walker, cond-mat/0512066 (2005).
[3] E. H. Rezayi and F. D. M. Haldane, Phys. Rev. Lett. **84** 4685 (2000).
[4] A. Emperador, E. Lipparini, and F. Pederiva, Phys. Rev. B **72**, 033306 (2005).
[5] J. K. Jain and R. K. Kamilla, Int. J. Mod. Phys. B **11**, 2621 (1997).
[6] H. Saarikoski, A. Harju, M. J. Puska, and R. M. Nieminen, Phys. Rev. Lett. **93**, 116802 (2004).
[7] One possibility to define ν of a particular *state* in QD is from the number of electrons on 0LL ($N_{\rm 0LL}$) as $\nu_{\rm 0LL} = 2N/N_{\rm 0LL}$. A second option is by Kinaret *et al.* [8] who defined the average filling factor as $\nu_{\rm avg} = N^2/2(N+L)$, where L is the total angular momentum. These two definitions differ especially in the low magnetic field range.
[8] J. M. Kinaret, Y. Meir, N. S. Wingreen, P. A. Lee, and X. G. Wen Phys. Rev. B **46**, 4681 (1992).
[9] M. Ciorga, A. Wensauer, M. Pioro-Ladriere, M. Korkusinski, J. Kyriakidis, A. S. Sachrajda, and P. Hawrylak, Phys. Rev. Lett. **88** 256804 (2002).
[10] M. Keller, U. Wilhelm, J. Schmid, J. Weis, K. v. Klitzing, and K. Eberl, Phys. Rev. B, **64**, 033302 (2001).
[11] K. Hitachi, M. Yamamoto, and S. Tarucha, unpublished.
[12] S. Tarucha, D. G. Austing, Y. Tokura, W. G. van der Wiel, and L. P. Kouwenhoven, Phys. Rev. Lett. **84**, 2485 (2000).
[13] M. Stopa, W. G. van der Wiel, S. De Franceschi, S. Tarucha, and L. P. Kouwenhoven, Phys. Rev. Lett. **91**, 046601 (2003).
[14] N. A. Bruce and P. A. Maksym, Phys. Rev. B **61**, 4718 (2000).
[15] M. P. Schwarz, D. Grundler, Ch. Heyn, D. Heitmann, D. Reuter, and A. Wieck, Phys. Rev. B **68**, 245315 (2003).